

### Abstract

A regular approach to accounting for initial correlations, which allows to go beyond the unrealistic random phase (initial product state) approximation in deriving the evolution equations, is suggested. An exact homogeneous equation for a two-time equilibrium correlation function for the dynamical variables of a subsystem interacting with a boson field (heat bath) is obtained. No conventional approximation like RPA or Bogoliubov's principle of weakening of initial correlations is used. The obtained equation takes into account the initial correlations in the kernel governing its evolution. The solution to this equation is found in the second order of the kernel expansion in the electron-phonon interaction, which demonstrates that generally the initial correlations influence the correlation function's evolution in time. It is shown that this influence vanishes on a large timescale. The developed approach is applied to the Fröhlich polaron and the low-temperature polaron mobility (which was under a long-time debate) is found with a correction due to initial correlations.

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# Influence of initial correlations on evolution of correlation function of a subsystem interacting with a quantum field (heat bath) and polaron mobility

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## 1 Introduction

Strict derivation of kinetic (irreversible) equations from the underlying reversible microscopic dynamics of the many-particle systems remains an important task of statistical physics due to its fundamental importance and various applications of these kinetic equations to the specific physical problems. Actually, to achieve this goal, several assumptions are conventionally used. The principal ones include the factorizing initial conditions (random phase approximation or "molecular chaos") corresponding to uncorrelated initial state and Bogoliubov's principle of weakening of initial correlations [1]. Such approximations, which, in fact, suggest that all initial (at the initial moment of time  $t_0$ ) correlations vanish on a large timescale, allow for obtaining the kinetic equations valid only on a large timescale. Thus, the main problem is to include initial correlations into consideration in order to obtain the equations which describe the system evolution on an arbitrary timescale and will, in particular, enable studying the influence of initial correlations on the relaxation process. The method which allows to include initial correlations into the kernel governing the evolution of the relevant part of the statistical operator of the many-body system (like gas or liquid) and obtain homogeneous generalized master equations valid on any timescale was developed in works [2, 3, 4, 5].

Another important case is a subsystem  $S$  of the total system interacting with an environment (a thermal bath)  $\Sigma$  of the remaining part of a whole system. In this case, the factorizing initial condition for the statistical operator of the whole system  $\rho(t)$

$$\rho(t_0) = \rho_S(t_0)\rho_\Sigma \quad (1)$$

is often used ( $\rho_S(t) = Tr_\Sigma \rho(t)$  is a subsystem statistical operator defined as a trace over a thermal bath states and  $\rho_\Sigma$  is the heat bath statistical operator). Such an approximation is incorrect in principle as it has been clearly pointed out by van Kampen [6]. It may, however, be expected, that according to Bogoliubov's principle of weakening of initial correlations, at a large timescale

$$t - t_0 \gg t_{cor}, \quad (2)$$

where  $t_{cor}$  is the correlation time for fluctuations in a heat bath, the initial correlations vanish and thus the condition (1) can be used.

The important (for quantum field theory and condensed matter physics) example of such a system is a particle interacting with a quantum field (heat bath). The electron-phonon system in a crystal is one of the realizations of such a system, which is important for practical applications. The notion of a polaron (a quasiparticle made of an electron and a cloud of phonons) introduced by Landau [7] has become crucial for understanding a crystal conductivity, especially in polar crystals [8]. Experimentally, the notion of the polaron is important to the understanding of a wide variety of materials, a few of which include the conductivity of semiconductors, high-temperature superconductors and the BEC with an immersed impurity atom (for more details see overview [9]). Recent experimental advances in the field of ultra-cold atoms offer new possibilities for experimental studies of polarons and have resulted in revived interest in the polaron problem.

The polaron ground-state (free energy) calculation is now done quite accurately over the complete interaction range [10]. At the same time, the Fröhlich polaron dynamics has been a matter of debate over a long time. Actually, three results on low-temperature polaron mobility have been obtained. Mainly, the discrepancy between the Kadanoff [11] and the Feynman-Hellwarth-Iddings-Platzman (FHIP) results [12] was discussed and only recently it has been understood [13]. There was also my result on polaron mobility, which is different from the two mentioned results [14]. It turned out, that neither the Kadanoff result nor the FHIP one are correct. Instead, the polaron mobility was found to agree with that of [14] (see [13] and for a detailed discussion [9]). It is worth mentioning that the result of the paper [14] was obtained in [13] independently and by using a method (truncation of the Liouville equation for the reduced Wigner distribution function) different from that of [14].

The polaron mobility can be calculated by different methods. The path integral approach of FHIP and the relaxation time approximation for the Boltzmann equation of Kadanoff were already mentioned. In [14], the Green-Kubo formula was employed for calculation of the conductivity tensor. The equilibrium current-current correlation function was calculated by the Green superoperator technique in [15]. In the papers [16] and [17], the closed Markovian equation for the density matrix of a subsystem interacting with a boson field (serving as a thermostat) was derived using the same Green superoperator method. As in the path integrals approach of FHIP, the bosonic degrees of freedom were eliminated exactly from the obtained equation. This equation for the density matrix was

applied in [17] to the polaron problem. In the paper [18], the closed equation for the Wigner function of a subsystem interacting with a heat bath and under the influence of inhomogeneous electric field was obtained and applied to the polaron problem.

However, in the paper [14], the initial correlations were disregarded for the purposes of calculating the current-current correlation function, i.e., the condition like (1) was used: the equilibrium distribution function in this correlation function (which in this case plays the role of the initial condition)  $\rho(\beta) = (Tr e^{-\beta H})^{-1} e^{-\beta H}$  ( $\beta = 1/k_B T$ ,  $H$  is the Hamiltonian of the whole electron+boson field system) was factorized (the correlation between an electron and the thermostat was omitted). The reason was that if we consider the long times  $t - t_0 \sim \tau_{rel} \gg \beta$  ( $\hbar = 1$ ,  $\tau_{rel}$  is a subsystem relaxation time,  $t_{cor} \sim \beta$ ), then the influence of initial correlations on an evolution process is small or vanishes (see also [6]). The same approximation was also used in papers [16, 17, 18], where the initial condition for the statistical operator of the whole system at the initial moment of time was selected (conventionally) as the factorized one (the product of the statistical operators of the subsystem and the thermal bath).

In this paper, by applying the projection operator technique, we obtain the exact closed homogeneous equation for the relevant part of the correlation function of a subsystem interacting with a boson field (thermostat). It includes the contribution of initial correlations ( $\rho(\beta)$  is accounted for in its exact form) to the kernel governing the evolution of a correlation function. The solution to this equation in the second order approximation in the electron-phonon interaction is found. It demonstrates that initial correlations influence the correlation function evolution in time on an arbitrary timescale. We show that this influence on the time dependence of the correlation function vanishes on a large timescale. The obtained equation is applied to the polaron problem and the low-temperature polaron mobility is calculated. In particular, small contribution of initial correlations to the result of [14] is found.

## 2 Exact equation for a subsystem correlation function accounting for initial correlations

We consider a subsystem  $S$  which interacts with a large equilibrium system (the heat bath  $\Sigma$ ). The Hamiltonian of the whole system  $S + \Sigma$  is

$$H = H_S + H_\Sigma + H_i, \quad (3)$$

where  $H_S$ ,  $H_\Sigma$  and  $H_i$  are the Hamiltonians of the subsystem, the Bose field (heat bath) and the subsystem-Bose field interaction, respectively.

The two-time correlation function for the arbitrary operators  $A$  and  $B$  related to the subsystem  $S$  interacting with a heat bath  $\Sigma$  can be written as

$$\langle A_S(t) B_S(0) \rangle = Tr_{S,\Sigma} [B_S(0) G_S(t, \beta)]. \quad (4)$$

Here,

$$G_S(t, \beta) = \rho(\beta) e^{iLt} A_S(0), \quad (5)$$

$Tr_{S,\Sigma}$  means taking a trace over the states of the whole system  $S + \Sigma$ , the averaging is performed with the equilibrium distribution of the whole system  $\rho(\beta) = (Tr e^{-\beta H}) e^{-\beta H}$ ,  $L$  is the Liouville superoperator acting on the arbitrary operator  $D$  according to the rules

$$LD = [H, D] = HD - DH, e^{iLt} D = e^{iHt} D e^{-iHt}, \hbar = 1, \quad (6)$$

and  $L = L_S + L_\Sigma + L_i$  in accordance with the Hamiltonian (3).

We will consider the dynamics of the correlation function (3) by splitting the function (5) into the relevant  $R_S(t, \beta)$  and irrelevant  $I_S(t, \beta)$  parts

$$R_S(t, \beta) = P G_S(t, \beta), I_S(t, \beta) = Q G_S(t, \beta) \quad (7)$$

by means of the projection operator

$$\begin{aligned} P(\dots) &= \rho_\Sigma(\beta) Tr_\Sigma(\dots), Q = 1 - P, P^2 = P, Q^2 = Q, PQ = 0, \\ \rho_\Sigma(\beta) &= (Tr_\Sigma e^{-\beta H_\Sigma}) e^{-\beta H_\Sigma}, \end{aligned} \quad (8)$$

where  $Tr_\Sigma$  means performing the trace over the states of the heat bath  $\Sigma$  and  $\rho_\Sigma(\beta)$  is the heat bath equilibrium distribution.

It is not difficult to see that the dynamics of the correlation function (4) is completely defined by the relevant part of  $G_S(t, \beta)$ , i.e.

$$\langle A_S(t) B_S(0) \rangle = Tr_{S,\Sigma} [B_S(0) R_S(t, \beta)]. \quad (9)$$

Thus, we need an evolution equation for the function  $R_S(t, \beta)$ . Using the identity  $P + Q = 1$ , (5) and (7), we have

$$\begin{aligned} \frac{\partial}{\partial t} R_S(t, \beta) &= iPL[R_S(t, \beta) + I_S(t, \beta)], \\ \frac{\partial}{\partial t} I_S(t, \beta) &= iQL[R_S(t, \beta) + I_S(t, \beta)]. \end{aligned} \quad (10)$$

The solution to the equation (10) for a complementary (irrelevant) function  $I_S(t, \beta)$  reads

$$\begin{aligned} I_S(t, \beta) &= i \int_0^{t-t_0} M_Q(\tau, \beta) QL R_S(t - \tau, \beta) d\tau + M_Q(t - t_0, \beta) I_S(t_0, \beta), \\ M_Q(t, \beta) &= \exp(iQLQt). \end{aligned} \quad (11)$$

Substituting this solution to the first equation of (10) and selecting the initial moment of time  $t_0 = 0$ , we obtain the following equation for the relevant function  $R_S(t, \beta)$

$$\begin{aligned} \frac{\partial}{\partial t} R_S(t, \beta) &= iPLPR_S(t, \beta) - PLQ \int_0^t M_Q(\tau, \beta) QL R_S(t - \tau, \beta) d\tau \\ &\quad + iPLQM_Q(t, \beta) I_S(0, \beta). \end{aligned} \quad (12)$$

This equation is closed but contains the inhomogeneous (last in (12)) term accounting for correlation between the subsystem  $S$  and the thermostat  $\Sigma$  at the initial moment of time. These initial correlations, as it follows from the definition (7), are given by

$$\begin{aligned} Q\rho(\beta) &= \rho(\beta) - P\rho(\beta) = \rho(\beta) - \rho_\Sigma(\beta)\rho_S(\beta), \\ \rho_S(\beta) &= Tr_\Sigma\rho(\beta), \end{aligned} \quad (13)$$

where  $\rho_S(\beta)$  is the reduced distribution function for a subsystem. If we disregard these initial correlations by approximating the distribution function  $\rho(\beta)$  in (5) as  $\rho(\beta) = \rho_S(\beta)\rho_\Sigma(\beta)$ , then the inhomogeneous term in (12)  $I_S(0, \beta) = 0$ . Such a factorization of the distribution function for a system under consideration was used in our earlier papers (mentioned in the Introduction), particularly in [14]. In this paper, we will not use this approximation and include the initial correlations into consideration.

Direct accounting for initial correlations by means of solving the inhomogeneous equation (12) for  $R_S(t, \beta)$  is not effective and may lead to the appearance of the growing with time terms in this solution (see, e.g. [1]). Instead, we will include the initial correlations term into the kernel governing the evolution in time of function  $R_S(t, \beta)$  and thus obtain the homogeneous evolution equation for this function. Moreover, the expansion of this equation kernel in a small parameter is, as a rule, more effective than the expansion of an equation itself. This approach is in line with that employed in works [2, 3, 4, 5]. However, the essential difference with these works is that in our case we have the explicit expression for initial correlations defined by the equilibrium distribution  $\rho(\beta)$  for the whole system  $S + \Sigma$ .

Thus, to convert Eq. (12) into the exact homogeneous equation, we use the following identity

$$e^{-\beta H} = e^{-\beta H_0} - \int_0^\beta d\lambda e^{-\lambda H_0} H_i e^{\lambda H} e^{-\beta H}, \quad (14)$$

where  $H_0 = H_S + H_\Sigma$ . Using (14) and taking into account that  $Qe^{-\beta H_0} = 0$ ,  $P + Q = 1$ ,  $e^{iLt}e^{-iLt} = 1$ , the irrelevant initial correlation term  $I_S(0, \beta) = QG_S(0, \beta) = Q\rho(\beta)A_S(0)$  can be then presented as

$$\begin{aligned} I_S(0, \beta) &= -C_Q(t, \beta)[R_S(t, \beta) + I_S(t, \beta)], \\ C_Q(t, \beta) &= \int_0^\beta d\lambda Qe^{-\lambda H_0} H_i e^{\lambda H} e^{-iLt}. \end{aligned} \quad (15)$$

As a result, we have two coupled equations (11) and (15) for  $I_S(t, \beta)$  and  $I_S(0, \beta)$ . Inserting the solution of these equations for the irrelevant initial correlations term  $I_S(0, \beta)$  into Eq. (12), we obtain the exact homogeneous equation for the

relevant function  $R_S(t, \beta)$  which we are looking for

$$\begin{aligned} \frac{\partial}{\partial t} R_S(t, \beta) &= iPL[1 - K_Q(t, \beta)][R_S(t, \beta) + i \int_0^t d\tau M_Q(\tau, \beta)QLPR_S(t - \tau, \beta)], \\ K_Q(t, \beta) &= M_Q(t, \beta)[1 + C_Q(t, \beta)M_Q(t, \beta)]^{-1}C_Q(t, \beta). \end{aligned} \quad (16)$$

Equation (16) is the main result of this section. It differs from the conventional Generalized Master Equations (see, e.g. [15]) for the relevant part of the correlation function (or statistical operator) by the modified time-local (first in the r.h.s. of (16)) term and non-Markovian (integral) term which now contain the contribution of initial correlations. This modification is defined by operator  $K_Q(t, \beta)$ . It is essential that this operator is proportional to the interaction  $H_i$ , which makes it conventional for expanding the kernel of Eq. (16) in the subsystem-heat bath interaction. If we put  $K_Q(t, \beta) = 0$  (disregard initial correlations), we obtain the equation for the relevant part of the distribution function (4), which was used in [14].

### 3 Electrons in a crystal interacting with bosons

First of all we are interested in the problem of a polaron mobility in a polar crystal. In this case,

$$H_S = T(\mathbf{p}), H_\Sigma = \sum_{\mathbf{k}} \omega_{\mathbf{k}} b_{\mathbf{k}}^+ b_{\mathbf{k}}, \quad (17)$$

where  $T(\mathbf{p})$  is the kinetic energy of the electron with momentum  $\mathbf{p}$ ,  $\omega_{\mathbf{k}}$  is the energy of the Boson field quantum (phonon) with the wave vector  $\mathbf{k}$  ( $\hbar = 1$ ),  $b_{\mathbf{k}}^+$ ,  $b_{\mathbf{k}}$  are the Bose-operators of the creation and annihilation of phonons, respectively. It is often sufficient to use the linear in Bose-operators interaction Hamiltonian

$$H_i = \sum_{\mathbf{k}} (V_{\mathbf{k}} e^{i\mathbf{k}r} b_{\mathbf{k}} + V_{\mathbf{k}}^* e^{-i\mathbf{k}r} b_{\mathbf{k}}^+), \quad (18)$$

where  $V_{\mathbf{k}}$  is an electron-phonon interaction coefficient and  $r$  is an electron radius-vector.

It is easy to see that for projection operator  $P$  (8) commutes with  $L_S$ , and

$$PL_SQ = QL_SP = 0, PL_\Sigma = L_\Sigma P = 0, PL_\Sigma Q = QL_\Sigma P = 0. \quad (19)$$

Moreover, for  $H_\Sigma$  and  $H_i$  defined by (17) and (18),

$$PL_iP = 0. \quad (20)$$

The properties (19), (20) allow for simplification of our basic equations (16) and (??).

The superoperators entering these equations can be expanded into the series with respect to the interaction  $H_i$ . For example,

$$[1 + C_Q(t, \beta)M_Q(t, \beta)]^{-1} = \sum_{n=0}^{\infty} (-1)^n [C_Q(t, \beta)M_Q(t, \beta)]^n. \quad (21)$$

The exponentials in the superoperators  $C_Q(t, \beta)$  and  $M_Q(t, \beta)$  can be also expanded in  $H_i$  or  $L_i$ . At weak subsystem-thermostat interaction, these series may be regarded as the perturbation theory expansions.

Taking into account (19), (20), we can rewrite Eq. (16) as

$$\begin{aligned} \frac{\partial}{\partial t} R_S(t, \beta) &= iPL_S R_S(t, \beta) - iPL_i K_Q(t, \beta) R_S(t, \beta) \\ &\quad - PL_i [1 - K_Q(t, \beta)] \int_0^t d\tau M_Q(\tau, \beta) L_i P R_S(t - \tau, \beta). \end{aligned} \quad (22)$$

It is seen from (22), that in the zero approximation in the interaction  $H_i$ ,

$$R_S(t - \tau, \beta) = \exp[iL_S(t - \tau)] R_S(0, \beta) = \exp(-iL_S\tau) R_S(t, \beta). \quad (23)$$

Assuming that the electron-phonon interaction is proportional to a small parameter, taking into account (19) - (23) and that  $C_Q(t, \beta)$  is proportional to  $H_i$ , we can convert Eq. (22) in the following time-local equation in the second order in  $H_i$  approximation for the kernel governing the evolution of  $R_S(t, \beta)$

$$\begin{aligned} \frac{\partial}{\partial t} R_S(t, \beta) &= [iPL_S P - PL_i \int_0^t d\tau e^{iL_0\tau} L_i e^{-iL_S\tau} P \\ &\quad - iPL_i e^{iL_0 t} \int_0^\beta d\lambda e^{-\lambda H_0} H_i e^{\lambda H_0} e^{-iL_0 t} P] R_S(t, \beta) \end{aligned} \quad (24)$$

The first two terms on the right-hand-side of Eq. (24) coincide with that of [14] but in this paper we do not restrict ourselves (at this stage) to the large times  $t \sim \tau_{rel} \gg t_0$  (at [14], the upper limit of integration over  $\tau$  was extended to infinity) where  $t_0 = \max(t_S, t_\Sigma)$  ( $t_S$  is the electron characteristic collision time, e.g. of the  $1/k_B T$  order;  $t_\Sigma$  is of the order of fluctuations correlation time in the heat bath, which is defined by the characteristic phonon frequency). The third term in the r.h.s. of (24) is absent in the corresponding equation of [14]. It defines the contribution of initial correlations which are treated here on the equal footing with collisions (given by the second term).

Equation (24) completely defines the evolution equation for the correlation function (9) in the second order in  $H_i$  approximation with accounting for initial correlations

$$\frac{\partial}{\partial t} \langle A_S(t) B_S(0) \rangle = Tr_{S,\Sigma} [B_S(0) \frac{\partial}{\partial t} R_S(t, \beta)]. \quad (25)$$



Having in mind the further application of this equation to the polaron mobility problem, let us take the subsystem operator  $B_S(0)$  dependent only on the momentum operator,  $B_S(0) = B_S(\mathbf{p})$ . Then, the trace over the subsystem (electron states) in (25) can be conveniently calculated using the eigenfunctions of  $H_S$  (17), i.e., the eigenfunctions  $|\mathbf{p}\rangle$  of the momentum operator. Therefore, we need to find  $\frac{\partial}{\partial t}R_S(t, \beta; \mathbf{p})$ , i.e., the equation (24) for the diagonal matrix element of  $\langle \mathbf{p}|R_S(t, \beta)|\mathbf{p}\rangle = R_S(t, \beta; \mathbf{p})$ .

It is not difficult to see that for  $H_S = T(\mathbf{p})$  the diagonal matrix element of the first term on the r.h.s. of (24)  $\langle \mathbf{p}|L_S R_S(t, \beta)|\mathbf{p}\rangle = 0$  (we used the rule (6)). Let us now consider the contribution of electron collisions with the bath quanta (phonons) to Eq. (24) (the second term on the r.h.s. of (24)). Applying consecutively the superoperators and projection operator  $P$  in this term to  $R_S(t, \beta)$ , making use of the rules (6), and taking into account that for the Hamiltonian, given by Eqs. (17), (18),

$$\begin{aligned} e^{iH_S t} b_{\mathbf{k}} e^{-iH_S t} &= e^{-i\omega_{\mathbf{k}} t} b_{\mathbf{k}}, e^{iH_S t} b_{\mathbf{k}}^+ e^{-iH_S t} = e^{i\omega_{\mathbf{k}} t} b_{\mathbf{k}}^+, \\ \langle b_{\mathbf{k}} b_{\mathbf{k}_1} \rangle_{\Sigma} &= 0, \langle b_{\mathbf{k}}^+ b_{\mathbf{k}_1}^+ \rangle_{\Sigma} = 0, \\ \langle b_{\mathbf{k}} b_{\mathbf{k}_1}^+ \rangle_{\Sigma} &= (1 + N_{\mathbf{k}}) \delta_{\mathbf{k}\mathbf{k}_1}, \langle b_{\mathbf{k}}^+ b_{\mathbf{k}_1} \rangle_{\Sigma} = N_{\mathbf{k}} \delta_{\mathbf{k}\mathbf{k}_1}, \\ \langle \dots \rangle_{\Sigma} &= Tr_{\Sigma}(\dots \rho_{\Sigma}), N_{\mathbf{k}} = [\exp(\beta\omega_{\mathbf{k}}) - 1]^{-1}, \end{aligned} \quad (26)$$

we obtain the collision term in (24) with

$$\begin{aligned} &\langle \mathbf{p}|PL_i \int_0^t d\tau e^{iL_0 \tau} L_i e^{-iL_S \tau} P R_S(t, \beta)|\mathbf{p}\rangle \\ &= 2 \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \left\{ \left[ \frac{\sin([T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) + \omega_{\mathbf{k}}]t)}{T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) + \omega_{\mathbf{k}}} (1 + N_{\mathbf{k}}) \right. \right. \\ &\quad \left. \left. + \frac{\sin([T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) - \omega_{\mathbf{k}}]t)}{T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) - \omega_{\mathbf{k}}} N_{\mathbf{k}} \right] R_S(t, \beta; \mathbf{p}) \right. \\ &\quad \left. - \left[ \frac{\sin([T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) - \omega_{\mathbf{k}}]t)}{T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) - \omega_{\mathbf{k}}} (1 + N_{\mathbf{k}}) \right. \right. \\ &\quad \left. \left. + \frac{\sin([T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) + \omega_{\mathbf{k}}]t)}{T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) + \omega_{\mathbf{k}}} N_{\mathbf{k}} \right] R_S(t, \beta; \mathbf{p} - \mathbf{k}) \right\}. \end{aligned} \quad (27)$$

In order to obtain (27), we also used that

$$\langle \mathbf{p}_1 | e^{\pm i\mathbf{k}\mathbf{r}} | \mathbf{p}_2 \rangle = \delta(\mathbf{p}_2 \pm \mathbf{k} - \mathbf{p}_1). \quad (28)$$

Note, that Eq. (27) is valid for arbitrary time  $t$ , in contrast to the corresponding collision term obtained in [14].

The diagonal matrix element of the third term in the r.h.s. of Eq. (24), which defines the contribution of initial correlations, can be calculated in the

same way. The result is

$$\begin{aligned}
& \langle \mathbf{p} | iPL_i e^{iL_0 t} \int_0^\beta d\lambda e^{-\lambda H_0} H_i e^{\lambda H_0} e^{-iL_0 t} P R_S(t, \beta) | \mathbf{p} \rangle \\
&= i \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \int_0^\beta d\lambda \{ [e^{i[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})+\omega_{\mathbf{k}}](t+i\lambda)} (1+N_{\mathbf{k}}) \\
&+ e^{i[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})-\omega_{\mathbf{k}}](t+i\lambda)} N_{\mathbf{k}}] R_S(t, \beta; \mathbf{p}) \\
&- [e^{-i[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})-\omega_{\mathbf{k}}](t+i\lambda)} (1+N_{\mathbf{k}}) \\
&+ e^{-i[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})+\omega_{\mathbf{k}}](t+i\lambda)} N_{\mathbf{k}}] R_S(t, \beta; \mathbf{p}-\mathbf{k}) \} \quad (29)
\end{aligned}$$

The integration over  $\lambda$  (which can be easily performed) is saved in (29) just for making this result more short in writing.

Inserting (27) and (29) in (25), we arrive at the following equation for the correlation function

$$\begin{aligned}
\frac{\partial}{\partial t} \langle A_S(t) B_S(0) \rangle &= Tr_\Sigma \int d\mathbf{p} B_S(\mathbf{p}) \frac{\partial}{\partial t} R_S(t, \beta; \mathbf{p}) \\
&= -Tr_\Sigma \int d\mathbf{p} B_S(\mathbf{p}) [\gamma_S(t, \beta; \mathbf{p}) + \gamma'_S(t, \beta; \mathbf{p})] R_S(t, \beta; \mathbf{p}), \quad (30)
\end{aligned}$$

where

$$\begin{aligned}
\gamma_S(t, \beta; \mathbf{p}) &= 2 \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{B_S(\mathbf{p}) - B_S(\mathbf{p}-\mathbf{k})}{B_S(\mathbf{p})} \\
&\times \{ (1+N_{\mathbf{k}}) \frac{\sin([T(\mathbf{p})-T(\mathbf{p}-\mathbf{k})-\omega_{\mathbf{k}}]t)}{T(\mathbf{p})-T(\mathbf{p}-\mathbf{k})-\omega_{\mathbf{k}}} \\
&+ N_{\mathbf{k}} \frac{\sin([T(\mathbf{p})-T(\mathbf{p}-\mathbf{k})+\omega_{\mathbf{k}}]t)}{T(\mathbf{p})-T(\mathbf{p}-\mathbf{k})+\omega_{\mathbf{k}}} \}, \\
\gamma'_S(t, \beta; \mathbf{p}) &= i \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{B_S(\mathbf{p}) - B_S(\mathbf{p}-\mathbf{k})}{B_S(\mathbf{p})} \\
&\times \{ (1+N_{\mathbf{k}}) e^{i[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})+\omega_{\mathbf{k}}]t} \frac{1 - e^{-[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})+\omega_{\mathbf{k}}]\beta}}{T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})+\omega_{\mathbf{k}}} \\
&+ N_{\mathbf{k}} e^{i[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})-\omega_{\mathbf{k}}]t} \frac{1 - e^{-[T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})-\omega_{\mathbf{k}}]\beta}}{T(\mathbf{p}-\mathbf{k})-T(\mathbf{p})-\omega_{\mathbf{k}}} \}. \quad (31)
\end{aligned}$$

The term  $\gamma'_S(t, \beta; \mathbf{p})$  is due to initial correlations and is valid, as well as  $\gamma_S(t, \beta; \mathbf{p})$ , for all  $t$  and temperature ( $\beta^{-1}$ ).

Thus, we have the following equation for function  $R_S(t, \beta; \mathbf{p})$ , which completely defines the correlation function (9),

$$\frac{\partial}{\partial t} \ln R_S(t, \beta; \mathbf{p}) = -[\gamma_S(t, \beta; \mathbf{p}) + \gamma'_S(t, \beta; \mathbf{p})]. \quad (32)$$

By integrating this equation over  $t$  (taking into account (31)), we obtain

$$R_S(t, \beta; \mathbf{p}) = R_S(0, \beta; \mathbf{p}) \exp\{-[\Gamma_S(t, \beta; \mathbf{p}) + \Gamma'_S(t, \beta; \mathbf{p})]\}, \quad (33)$$

where

$$\begin{aligned} \Gamma_S(t, \beta; \mathbf{p}) &= \int_0^t \gamma_S(\tau, \beta; \mathbf{p}) d\tau = 2 \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{B_S(\mathbf{p}) - B_S(\mathbf{p} - \mathbf{k})}{B_S(\mathbf{p})} \\ &\times \left\{ (1 + N_{\mathbf{k}}) \frac{1 - \cos([T(\mathbf{p}) - T(\mathbf{p} - \mathbf{k}) - \omega_{\mathbf{k}}]t)}{[T(\mathbf{p}) - T(\mathbf{p} - \mathbf{k}) - \omega_{\mathbf{k}}]^2} \right. \\ &\left. + N_{\mathbf{k}} \frac{1 - \cos([T(\mathbf{p}) - T(\mathbf{p} - \mathbf{k}) + \omega_{\mathbf{k}}]t)}{[T(\mathbf{p}) - T(\mathbf{p} - \mathbf{k}) + \omega_{\mathbf{k}}]^2} \right\}, \\ \Gamma'_S(t, \beta; \mathbf{p}) &= \int_0^t \gamma'_S(\tau, \beta; \mathbf{p}) d\tau = \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{B_S(\mathbf{p}) - B_S(\mathbf{p} - \mathbf{k})}{B_S(\mathbf{p})} \\ &\times \left\{ (1 + N_{\mathbf{k}}) [e^{i[T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) + \omega_{\mathbf{k}}]t} - 1] \frac{1 - e^{-[T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) + \omega_{\mathbf{k}}]\beta}}{[T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) + \omega_{\mathbf{k}}]^2} \right. \\ &\left. + N_{\mathbf{k}} [e^{i[T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) - \omega_{\mathbf{k}}]t} - 1] \frac{1 - e^{-[T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) - \omega_{\mathbf{k}}]\beta}}{[T(\mathbf{p} - \mathbf{k}) - T(\mathbf{p}) - \omega_{\mathbf{k}}]^2} \right\}, \\ R_S(0, \beta; \mathbf{p}) &= \rho_{\Sigma}(\beta) < \mathbf{p} | \rho_S(\beta) A_S(0) | \mathbf{p} >, \end{aligned} \quad (34)$$

If the subsystem operator  $A_S(0)$  depends only on the electron momentum  $\mathbf{p}$ , then the initial value

$$R_S(0, \beta; \mathbf{p}) = \rho_{\Sigma}(\beta) A_S(\mathbf{p}) \rho_S(\beta; \mathbf{p}), \quad (35)$$

where  $A_S(\mathbf{p}) = < \mathbf{p} | A_S(0) | \mathbf{p} >$ ,  $\rho_S(\beta; \mathbf{p}) = < \mathbf{p} | \rho_S(\beta) | \mathbf{p} >$ .

Finally, the considered correlation function for electron momentums in the second order in the small electron-boson field (thermostat) interaction is

$$< A_S(t) B_S(0) > = \int d\mathbf{p} \rho_S(\beta; \mathbf{p}) A_S(\mathbf{p}) B_S(\mathbf{p}) \exp\{-[\Gamma_S(t, \beta; \mathbf{p}) + \Gamma'_S(t, \beta; \mathbf{p})]\}, \quad (36)$$

where the relaxation functions  $\Gamma_S(t, \beta; \mathbf{p})$  and  $\Gamma'_S(t, \beta; \mathbf{p})$  are given by (34) and the function  $\Gamma'_S(t, \beta; \mathbf{p})$  defines the contribution of initial correlations. Thus, we have obtained the solution for the electron momentum-momentum correlation function in the second order in the electron-phonon interaction, which shows, that generally, the damping process is affected by initial correlations because  $\Gamma'_S(t, \beta; \mathbf{p})$  depends on time.

Although the obtained result, given by Eq. (33), is valid for the whole time range, there are some characteristic times in the problem under consideration. When the subsystem-boson field interaction is small, we can introduce the following time hierarchy

$$\tau_{rel} \gg t_0. \quad (37)$$

Here  $\tau_{rel}$  is of the order of the electron relaxation time due to the electron-bath interaction,  $t_0 = \max(t_S, t_\Sigma)$ , where  $t_S$  is characteristic time of electron's collisions (e.g.,  $t_S \sim 1/k_B T$ ) and  $t_\Sigma$  is the characteristic time of correlation of the thermostat fluctuations. It is instructive to consider the important large timescale  $t \sim \tau_{rel} \gg t_0$  (in fact, it is possible to take the limit  $t \rightarrow \infty$ ). In this case, the relaxation functions (34) acquire more simple form

$$\begin{aligned}\Gamma_S(t, \beta; \mathbf{p}) &= \tau_{rel}^{-1}(\beta, \mathbf{p}) |t|, \Gamma'_S(t, \beta; \mathbf{p}) = i \frac{1}{2} \tau_{rel}^{-1}(\beta, \mathbf{p}) \beta, \\ \tau_{rel}^{-1}(\beta, \mathbf{p}) &= 2\pi \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \frac{B_S(\mathbf{p}) - B_S(\mathbf{p} - \mathbf{k})}{B_S(\mathbf{p})} \\ &\times \{(1 + N_{\mathbf{k}}) \delta[T(\mathbf{p}) - T(\mathbf{p} - \mathbf{k}) - \omega_{\mathbf{k}}] + N_{\mathbf{k}} \delta[T(\mathbf{p}) - T(\mathbf{p} - \mathbf{k}) + \omega_{\mathbf{k}}]\}, \\ &t \gg t_0.\end{aligned}\tag{38}$$

To obtain (38), we have used the definitions

$$\begin{aligned}\lim_{t \rightarrow \infty} \frac{\sin \omega t}{\omega} &= \pi \delta(\omega), \\ \lim_{t \rightarrow \infty} \frac{1 - \cos \omega t}{\omega^2} &= \pi \delta(\omega) |t|.\end{aligned}\tag{39}$$

Note, that the relaxation function  $\Gamma'_S(t, \beta; \mathbf{p})$  ceases to depend on time. It means that on the large timescale the initial correlations do not influence the damping of the correlation function in time. Thus, on the timescale  $t \sim \tau_{rel} \gg t_0$ , the correlation function (36) is

$$\begin{aligned}< A_S(t) B_S(0) > = \int d\mathbf{p} \rho_S(\beta; \mathbf{p}) A_S(\mathbf{p}) B_S(\mathbf{p}) \exp[-\frac{i}{2} \tau_{rel}^{-1}(\beta, \mathbf{p}) \beta] \exp[-\tau_{rel}^{-1}(\beta, \mathbf{p}) |t|], \\ &t \sim \tau_{rel} \gg t_0.\end{aligned}\tag{40}$$

One can see, that on the large timescale the considered correlation function damps exponentially with time. In addition, there is the factor  $\exp[-\frac{i}{2} \tau_{rel}^{-1}(\beta, \mathbf{p}) \beta]$  describing the contribution of initial correlations. This factor is absent in the paper [14], where the consideration is restricted by the condition  $\tau_{rel}^{-1} \beta \ll 1$ , when this factor is approximately equal to unity. In the given paper, we take into consideration the initial correlations and are able to calculate the corresponding corrections to the earlier obtained results.

## 4 Polaron mobility

According to the Kubo theory of linear response, the dissipative part of the conductivity tensor is given by the following formula

$$\begin{aligned}\text{Re } \sigma_{\mu\nu}(\omega) &= \frac{1}{E_\beta(\omega)} \int_0^\infty \psi_{\mu\nu}(t) \cos(\omega t) dt, \\ E_\beta(\omega) &= \frac{\omega}{2} \coth \frac{\beta\omega}{2}, \\ \psi_{\mu\nu}(t) &= \frac{1}{2} \langle j_\mu(t) j_\nu(0) + j_\nu(0) j_\mu(t) \rangle.\end{aligned}\quad (41)$$

Here,  $j_\mu(t) = e^{iHt} j_\mu(0) e^{-iHt}$  is the  $\mu$ -component of the current operator in the Heisenberg representation,  $H$  is the Hamiltonian in the absence of an electric field, i.e. the Hamiltonian given by Eqs. (17) and (18). Note, that  $\langle j_\nu(0) j_\mu(t) \rangle = \langle j_\nu(-t) j_\mu(0) \rangle$ .

Let us consider the Fröhlich polaron in the unit system with  $\hbar = m^* = \omega_0 = 1$ , where  $m^*$  is an electron effective mass and  $\omega_0$  is the crystal optical mode frequency. Then,

$$\begin{aligned}H_S &= T(\mathbf{p}) = \frac{\mathbf{p}^2}{2}, H_\Sigma = \sum_{\mathbf{k}} b_{\mathbf{k}}^+ b_{\mathbf{k}}, H_i = \sum_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} b_{\mathbf{k}} + h.c., \\ V_{\mathbf{k}} &= 2^{3/4} \pi^{1/2} \alpha^{1/2} / V^{1/2} k,\end{aligned}\quad (42)$$

where  $\alpha$  is the dimensionless constant of the electron-phonon interaction and  $V$  is the system's volume. Now, the above obtained results for the correlation function can be directly applied to the calculation of the polar crystal conductivity and the Fröhlich polaron mobility. Since  $j_\mu(t) = ev_\mu(t)$  ( $e$  is the electron charge,  $v_\mu(t)$  is the velocity operator), we need the velocity-velocity correlation function  $\langle v_\mu(t) v_\nu(0) \rangle$ , which can be calculated from Eq. (36) for arbitrary timescale. In particular, using Eq. (40), we get for large timescale  $t \gg t_0$

$$\langle v_\mu(t) v_\nu(0) \rangle = \int d\mathbf{p} \rho_S(\beta; \mathbf{p}) v_\mu(\mathbf{p}) v_\nu(\mathbf{p}) \exp\left[-\frac{i}{2} \tau_{rel}^{-1}(\beta, \mathbf{p}) \beta\right] \exp\left[-\tau_{rel}^{-1}(\beta, \mathbf{p}) |t|\right], t \gg t_0, \quad (43)$$

where  $\tau_{rel}(\beta, \mathbf{p})$  now is determined by (38) with  $B_S(\mathbf{p}) = v_\nu(\mathbf{p}) = \partial T(\mathbf{p}) / \partial p_\nu$ , and  $V_{\mathbf{k}}$  and  $T(\mathbf{p})$  are given by (42). This formula can be used for calculation of the low frequency conductivity (41), when  $\omega \ll t_0^{-1}$ .

To simplify the consideration, let us consider the isotropic case, when  $\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma$  (non-diagonal components are equal to zero). Then, the relaxation frequency (38) for the correlation function  $\langle v_z(t) v_z(0) \rangle$  after integration

over  $k$  acquires the form (see also [14])

$$[\tau_{rel}^{-1}(\beta, \mathbf{p})]_z = \Gamma_z(\beta, \mathbf{p}) = \frac{\alpha}{\sqrt{2\pi}p_z}[(1 + N_0) \int_{(p \cos \theta_1 > \sqrt{2})} d\Omega \cos \theta \frac{2p \cos \theta_1}{\sqrt{p^2 \cos^2 \theta_1 - 2}} + N_0 \int d\Omega \cos \theta \frac{p \cos \theta_1}{\sqrt{p^2 \cos^2 \theta_1 + 2}}]. \quad (44)$$

Here,  $N_0 = (e^\beta - 1)^{-1}$ ,  $d\Omega = d\varphi \sin \theta d\theta$ , the angles  $\varphi$  and  $\theta$  define the direction of the wave vector  $\mathbf{k}$ , and  $\theta_1$  is the angle between  $\mathbf{p}$  and  $\mathbf{k}$ , which is related to  $\varphi$  and  $\theta$  as

$$p \cos \theta_1 = \sin \theta \cos \varphi p_x + \sin \theta \sin \varphi p_y + \cos \theta p_z. \quad (45)$$

The area of integration in the first integral is defined by the condition of the integrand positive value.

It is interesting to consider the low temperature case  $\beta \gg 1$  ( $k_B T \ll \omega_0$ ), which was under debate for more than thirty years (see Introduction and [9]). As was mentioned, the correct low-temperature polaron mobility, which agrees with the experiment, was obtained in [14]. In the present paper, we are able to consider the influence of initial correlations on the low-temperature polaron mobility. It is seen from (36) and (42), that at low temperature  $\beta \gg 1$ , the main contribution to correlation function comes from the area of small electron momenta  $p^2 \ll 2$ . Thus, in this case, the first term in the relaxation frequency (44), which corresponds to the emitting of phonon by electron, vanishes due to impossibility to satisfy the energy and momentum conservation law. In the second term of (44), we can omit  $p^2 \cos^2 \theta_1$  in the denominator. As a result, this term, which describes the process of the phonon adsorption by an electron, after integration reduces to

$$\Gamma_z(\beta, \mathbf{p}) = \Gamma^0 = \frac{2}{3} \alpha N_0, p^2 \ll 2. \quad (46)$$

Thus, at small momenta, the relaxation frequency does not depend on  $\mathbf{p}$ .

Now, we can calculate from (41) the low-temperature electron conductivity of the Fröhlich polaron. To do that, we also need the correlation function  $\langle v_z(0)v_z(t) \rangle = \langle v_z(-t)v_z(0) \rangle$ . It is not difficult to see from (34) and (39), that this correlation function at  $t \gg t_0$  is given by (43) with the substitution  $\beta \rightarrow -\beta$ . Substituting (43) with the relaxation frequency (46) and the corresponding expression for  $\langle v_z(-t)v_z(0) \rangle$  into (41), we obtain the following low frequency conductivity of the Fröhlich polaron

$$\sigma(\omega) = ne^2 \langle v_z^2 \rangle \beta \frac{\Gamma^0}{\omega^2 + (\Gamma^0)^2} \cos(\Gamma^0 \beta), \omega \ll \beta^{-1} \ll 1, \quad (47)$$

where  $n$  is the electron concentration,  $\langle v_z^2 \rangle = \int d\mathbf{p} \rho_S(\beta; \mathbf{p}) v_z^2(\mathbf{p})$ .

Thus, in the considered range of the parameters, we have the Drude formula for conductivity. The low-temperature polaron mobility, as it follows from (46)

and (47), is

$$\begin{aligned}\mu &= \sigma(0)/ne = \mu_0 - \Delta\mu, \beta \gg 1, \\ \mu_0 &= \frac{3e}{2\alpha}e^\beta, \Delta\mu = \frac{e}{3}\alpha\beta^2e^{-\beta},\end{aligned}\tag{48}$$

where we used, that with a good accuracy  $\langle v_z^2 \rangle = \beta^{-1}$  (in the adopted unit system), and expanded  $\cos(\Gamma^0\beta)$  up to the second power in the small term  $\Gamma^0\beta \ll 1$ .

The obtained result shows, that accounting for initial correlations results in the very small correction  $\Delta\mu \ll \mu_0$  to the expression for the low-temperature polaron mobility  $\mu_0$  found in [14] and confirmed later in [13] (see also discussion in [9]). Anyway, this correction is important, since we have not used any unrealistic approximation for the initial state of the system under consideration. However, it should be kept in mind, that the result (48) is valid for  $\omega = 0$ , i.e. for a large timescale ( $t \rightarrow \infty$ ) when, as was mentioned earlier, the initial correlations do not influence the time relaxation process. For shorter times (larger frequencies  $\omega$ ) the initial correlations can influence the damping of the correlation function in time (see Eq. (36)). Thus, it is of principal importance to have a comprehensive approach to calculation of contribution of initial correlations to the evolution of the subsystem, which has been suggested in this paper.

## 5 Conclusion

We have derived the exact equation (16), which defines the evolution in time of the two-time correlation function (4) of a subsystem interacting with a boson field (a heat bath) and accounts for initial correlations. The obtained equation provides the regular procedure for including into consideration the influence of initial correlations (ignored as a rule) on the evolution process. Initial correlations enter the kernel governing the correlation function evolution on an equal footing with the terms defining the collisions of a subsystem with the heat bath excitations. In the second order of the particle-bath interaction expansion of the kernel governing the evolution of the electron momentum-momentum correlation function, we have obtained the solution to this correlation function (Eq. (36)) on an arbitrary timescale. It shows that generally the initial correlations influence the evolution in time process. However, on a large timescale, this influence vanishes (in accordance with Bogoliubov's principal of initial correlations) and the initial correlations contribute only to the amplitude of the exponential damping of the corresponding dynamical variable (see Eq. (40)). As an application, the low-temperature Fröhlich polaron mobility is considered. We found a small correction to our earlier result [14] which shows that initial correlations slightly reduce the low-temperature polaron mobility.

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